

2-Benzyl-2,3-dihydro-1H-pyrrolo[3,4-c]pyridine  
368441-96-7 | DTXSID50364048

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 2.49

Global applicability domain: Inside

Local applicability domain index: 5.51e-01

Confidence level: 5.10e-01

Nearest Neighbors from the Training Set

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Isothiocyanic acid, p-dimethylaminophenyl ester  
**Measured:** 3.96  
**Predicted:** 1.81

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3-(1-Piperaziny)-1,2-benzisothiazole  
**Measured:** 2.14  
**Predicted:** 1.50

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1-(4-Chlorophenyl)piperazine  
**Measured:** 2.01  
**Predicted:** 1.74

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1-(3-Chlorophenyl)piperazine  
**Measured:** 2.11  
**Predicted:** 1.74

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1-(2-Chlorophenyl)piperazine  
**Measured:** 2.13  
**Predicted:** 1.78